

Problem with the derivation of the Navier-Stokes equation by means of Zwanzig-Mori technique: Correction and solution

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Abstract

The derivation of the Navier-Stokes equation starting from the Liouville equation using projector techniques yields a friction term which is nonlinear in the velocity. As has been explained in the 1. version of this paper, when the second-order part of the term is non-zero, this leads to an incorrect formula for the equation.

In this 2. version, it is shown that the problem is due to an inadequate treatment of the correlation function K_2 . Repeating the calculation leads to zero second-order part. The Navier-Stokes equation is correctly derived by projection operator technique.

1 Introduction

The derivation of hydrodynamic equations by Zwanzig-Mori technique is a method well-established in the literature. In version 1 of this paper, the author reported a problem which occurred when the Navier-Stokes order of the momentum equation is considered: As is well known, the non-dissipative part shows to be of second order in the fluid velocity, \mathbf{u} . The dissipative part is also non-linear in \mathbf{u} . In order to obtain the correct form of the Navier-Stokes equation, it is necessary for the second-order part of the dissipation term to vanish. As far as the author knows, this aspect has not been investigated earlier. The calculation in version 1 yielded a second-order part different from zero.

In the present version it is shown that the problem resulted from an incomplete formula for the correlation function K_2 . Actually, the second-order term is zero. Thus, the Navier-Stokes equation is correctly derived by projection operator technique.

2 Hydrodynamic equations

For the basic definitions of microscopic variables, readers are referred to [1]. In order to keep the paper reasonably self-contained, the results of the Zwanzig-Mori analysis are copied from there. The analysis is for incompressible constant density/temperature processes. The hydrodynamic momentum equation is a specialization of the general mean value equation (3.1):

$$\rho \left(\frac{du_a}{dt} + u_c \nabla_c u_a \right) = -\nabla_a P + D_a \quad (2.1)$$

In (3.15) this equation is given for stationary processes. Latin indices run from 1 to 3. ρ is the fluid density; \mathbf{u} as well as the pressure P and the dissipative force \mathbf{D} depend on space and time. For the latter the formula is obtained:

$$D_a(\mathbf{x}, t) = \beta \nabla_c \int_0^t dt' \int d\mathbf{x}' R_{abcd}(\mathbf{x}, t, \mathbf{x}', t') \nabla'_d u_b(\mathbf{x}', t') \quad (2.2)$$

with the kernel function:

$$R_{abcd}(\mathbf{x}, t, \mathbf{x}', t') = \langle [\mathcal{G}(t', t) \hat{s}_{ac}(\mathbf{x}, t)] \hat{s}_{bd}(\mathbf{x}', t') \rangle_{L, t'} \quad (2.3)$$

β is the inverse kinetic temperature. $\langle \rangle_{L,t}$ denotes the expectation with respect to local equilibrium, cf. [1] (3.4) to (3.6). \hat{s}_{ac} is the projected momentum flux density:

$$\hat{s}_{ac}(\mathbf{x}, t) = (1 - \mathcal{P}(t))s_{ac}(\mathbf{x}) \quad (2.4)$$

s_{ac} is the momentum flux density. $\mathcal{P}(t)$ is the Zwanzig-Mori projection operator; for any phase space function g , it is defined:

$$\mathcal{P}g = \langle g \rangle_L + \langle g \delta a \rangle_L * \langle \delta a \delta a \rangle_L^{-1} * \delta a \quad (2.5)$$

For shortness, the time parameters have been omitted here. $*$ denotes an operation which consists of a product, a summation over 5 index values and a space integration. a are the microscopic densities of the conserved quantities. $\delta a = a - \langle a \rangle_L$. $\langle \rangle^{-1}$ denotes the inverse matrix. $\mathcal{G}(t', t)$ is a time-ordered exponential operator:

$$\mathcal{G}(t', t) = \exp_{-} \left\{ \int_{t'}^t dt'' \mathcal{L}(1 - \mathcal{P}(t'')) \right\} \quad (2.6)$$

\mathcal{L} is the Liouville operator, cf. [1] (2.4).

3 2^{nd} order term of the friction force

In this paper, we consider the second-order velocity approximation of the friction Term **D**. This should not be confused with the second-order wave number approximation of the linear part of **D** which leads to the well-known Stokes form of that term. This latter approximation is not considered here.

As is explained in [1], the 2^{nd} order part $\mathbf{D}^{(2)}$ of the dissipative force is obtained from (2.2) by inserting the linear part $R^{(1)}$ of the kernel function given by [1] (4.1), (4.2). These formulas have to be generalized for time-dependent processes:

$$R_{abcd}^{(1)}(\mathbf{x}, \mathbf{x}', t, t') = -\beta \int_0^\infty dt'' \int d\mathbf{x}'' \frac{\delta R_{abcd}(\mathbf{x}, \mathbf{x}', t, t')}{\delta b_e(\mathbf{x}'', t'')} \big|_{\mathbf{u}=0} u_e(\mathbf{x}'', t'') \quad (3.1)$$

$b_e = -\beta u_e$ is the momentum part of the conjugated parameters in the formula for the local equilibrium probability density, see [1] (3.6). The functional derivative is calculated in the appendix.

The second-order term of the friction force consists of a parametric and a functional part:

$$D_2 = D_{2p} + D_{2f} \quad (3.2)$$

When the parametric part of the derivative (A.7) is inserted into (3.1), and the result is introduced into (2.2), one obtains the parametric part of the second-order friction force. We find:

$$(D_{2p})_a(\mathbf{x}, t) = \beta^2 \nabla_c \int d\mathbf{x}' \int d\mathbf{x}'' \int_0^t dt' \langle [e^{(1-\mathcal{P}_0)\mathcal{L}(t-t')} (\hat{s}_0)_{ac}(\mathbf{x})] (\hat{s}_0)_{bd}(\mathbf{x}') p_e(\mathbf{x}'') \rangle_0 u_e(\mathbf{x}'', t') \nabla'_d u_b(\mathbf{x}', t') \quad (3.3)$$

$\langle \rangle_0$ denotes total equilibrium expectation; \hat{s}_0 is the flux variable projected with $(1 - \mathcal{P}_0)$; \mathcal{P}_0 is the total equilibrium counterpart of \mathcal{P} (2.5). - If one inserts the 4^{th} part of the derivative (A.16) into (3.1), one obtains the functional part of the friction force:

$$(D_{2f})_a(\mathbf{x}, t) = \beta^2 \nabla_c \int d\mathbf{x}' \int d\mathbf{x}'' \int_0^t dt' \int_{t'}^t dt'' \times \\ \times \left\langle \left[\frac{d}{dt'} e^{(1-\mathcal{P}_0)\mathcal{L}(t''-t')} \mathcal{P}_0 p_e(\mathbf{x}'') e^{(1-\mathcal{P}_0)\mathcal{L}(t-t'')} (\hat{s}_0)_{ac}(\mathbf{x}) \right] (\hat{s}_0)_{bd}(\mathbf{x}') \right\rangle_0 u_e(\mathbf{x}'', t'') \nabla'_d u_b(\mathbf{x}', t') \quad (3.4)$$

It is necessary to derive formulas for the appearing correlation functions in order to get a definite result. - We begin with transferring the formulas into Fourier space. In addition, within the correlation formula, we switch to orthonormal variables h_e , r_{ac} , \hat{r}_{ac} (see [1] (4.7)).

The hydrodynamic velocity varies over much larger time intervals than the correlation functions. Therefore, a Markovian approximation of the process is applied which results in the approximation for the kernel function $f(t)$ in the integrals: $f(t) \rightarrow \delta(t) \int_0^\infty dt' f(t')$. For the parametric part, we obtain:

$$(D_{2p})_1(t) = \beta^{\frac{1}{2}} \rho^{\frac{3}{2}} \frac{1}{(2\pi)^6} \int d\mathbf{q} \int d\mathbf{q}' (N_p)_{123} u_2(t) u_3(t) \quad (3.5)$$

$$(N_p)_{123} = \int_0^\infty dt' \langle [e^{(1-\mathcal{P}_0)\mathcal{L}t'} (i\mathbf{k}\hat{r})_1] (i\mathbf{q}\hat{r})_2^* h_3^* \rangle_0 \quad (3.6)$$

Number indices are introduced which have been used by many authors. The number is a combination of an index and a wave number. Certain numbers are reserved for a specific wave number, as is shown in the following table:

$$\begin{aligned} \mathbf{k} &: 1, 4, 7, \dots \\ \mathbf{q} &: 2, 5, 8, \dots \\ \mathbf{q}' &: 3, 6, 9, \dots \end{aligned}$$

Number indices appearing pairwise include a summation over the original indices; on the other hand, wave number integration will always be shown explicitly. In (3.6), $(i\mathbf{k}\hat{r})_1$ is written for $i\mathbf{k}_d\hat{r}_{1d}$. - N_p is identical with the quantity N in [1] (4.10), which is calculated there. The result (4.27) is the "reduced" form of the kernel function which means that the factor $(2\pi)^3\delta(\mathbf{k} - \mathbf{q} - \mathbf{q}')$ is excluded. The full formula reads

$$(N_p)_{123} = (2\pi)^3\delta(\mathbf{k} - \mathbf{q} - \mathbf{q}') \frac{1}{2} i k_d S_{123d} \quad (3.7)$$

Details of the matrix S are not needed and are therefore not repeated here. - (3.4) changes to:

$$\begin{aligned} (D_{2f})_1(t) &= -\beta^{\frac{1}{2}} \rho^{\frac{3}{2}} \frac{1}{(2\pi)^6} \int d\mathbf{q} \int d\mathbf{q}' k_c q_d \int_0^t dt' \int_{t'}^t dt'' \times \\ &\times \langle [\frac{d}{dt'} e^{(1-\mathcal{P}_0)\mathcal{L}(t''-t')} \mathcal{P}_0 h_3^* e^{(1-\mathcal{P}_0)\mathcal{L}(t-t'')} \hat{r}_{1c}] \hat{r}_{2d}^* \rangle_0 u_2(t') u_3(t'') \end{aligned} \quad (3.8)$$

The projection \mathcal{P}_0 in the correlation is performed:

$$\begin{aligned} (D_{2f})_1(t) &= -\beta^{\frac{1}{2}} \rho^{\frac{3}{2}} \frac{1}{(2\pi)^6} \int d\mathbf{q} \int d\mathbf{q}' \int_0^t dt' \int_{t'}^t dt'' \times \\ &\times \langle [e^{(1-\mathcal{P}_0)\mathcal{L}(t-t'')} (i\mathbf{k}\hat{r})_1] h_2^* h_3^* \rangle_0 \langle [\frac{d}{dt'} e^{(1-\mathcal{P}_0)\mathcal{L}(t''-t')} h_2] (i\mathbf{q}\hat{r})_5^* \rangle_0 u_5(t') u_3(t'') \end{aligned} \quad (3.9)$$

$\tilde{\langle} \rangle_0$ denotes the 3-point-correlation without the factor $(2\pi)^3\delta(\mathbf{k} - \mathbf{q} - \mathbf{q}')$, which we call the reduced correlation function. - Finally, symbols are introduced for the correlations appearing in (3.6):

$$(D_{2f})_1(t) = -\beta^{\frac{1}{2}} \rho^{\frac{3}{2}} \frac{1}{(2\pi)^6} \int d\mathbf{q} \int d\mathbf{q}' \int_0^t dt'' \int_0^{t''} dt' (K_3)_{123}(t-t'') \frac{d(K_2)_{25}(t''-t')}{dt'} u_3(t'') u_5(t') \quad (3.10)$$

$$(K_3)_{123}(t) = \langle [e^{(1-\mathcal{P}_0)\mathcal{L}t} (i\mathbf{k}\hat{r})_1] h_2^* h_3^* \rangle_0 \quad (3.11)$$

$$(K_2)_{25}(t) = \langle [e^{(1-\mathcal{P}_0)\mathcal{L}t} h_2] (i\mathbf{q}\hat{r})_5^* \rangle_0 \quad (3.12)$$

4 Correlation function K_2

We start the investigation of K_2 by calculating its initial value:

$$(K_2)_{25}(0) = \langle h_2 (i\mathbf{q}\hat{r})_5^* \rangle_0 = \langle [(1-\mathcal{P})h_2] (i\mathbf{q}\hat{r})_5^* \rangle_0 = 0 \quad (4.1)$$

Here we have used the general properties $\langle f(1-\mathcal{P})g \rangle_0 = \langle [(1-\mathcal{P})f](1-\mathcal{P})g \rangle_0$ and $(1-\mathcal{P})h = 0$. Next we derive a relation between K_2 and correlation functions which are defined with the non-projected exponential operator $e^{\mathcal{L}t}$. For K_2 , we use the relation:

$$(i\mathbf{k}\hat{r})_1 = -\dot{h}_1 - i\omega_{14}h_4 \quad (4.2)$$

We obtain the decomposition:

$$\begin{aligned}
(K_2)_{25}(t) &= -\langle [e^{(1-\mathcal{P}_0)\mathcal{L}t} h_2] \dot{h}_5^* \rangle_0 + i\omega_{58} \langle [e^{(1-\mathcal{P}_0)\mathcal{L}t} h_2] h_8^* \rangle_0 \\
&\quad - (K_{21})_{25}(t) + i\omega_{58} (K_{22})_{28}(t)
\end{aligned} \tag{4.3}$$

$\omega_{25} = \langle (\mathbf{q}\hat{r})_2 h_5^* \rangle_0$, and the symbols in the second row are denotations for the quantities in the first. We use the operator identity [1] (4.11):

$$e^{(1-\mathcal{P}_0)\mathcal{L}t} = e^{\mathcal{L}t} - \int_0^t dt' e^{\mathcal{L}t'} \mathcal{P}_0 \mathcal{L} e^{(1-\mathcal{P}_0)\mathcal{L}(t-t')} \tag{4.4}$$

Application to K_{21} yields:

$$\begin{aligned}
(K_{21})_{25}(t) &= - \int_0^t dt' \langle [e^{\mathcal{L}t'} \mathcal{P}_0 \mathcal{L} e^{(1-\mathcal{P}_0)\mathcal{L}(t-t')} h_2] \dot{h}_5^* \rangle_0 + \langle [e^{\mathcal{L}t} h_2] \dot{h}_5^* \rangle_0 \\
&= - \int_0^t dt' (K_{21})_{28}(t-t') \frac{d(C_2)_{85}(t')}{dt'} - \frac{d(C_2)_{25}(t)}{dt}
\end{aligned} \tag{4.5}$$

This is an integral equation for K_{21} in terms of the non-projected duple correlation $(C_2)_{25}(t) = \langle [e^{\mathcal{L}t} h_2] h_5^* \rangle_0$. $(C_2)_{\tilde{}}$ means (C_2) without the factor $(2\pi)^3 \delta(\mathbf{k} - \mathbf{q})$, which we call the reduced form of the two-point correlation. C_2 obeys the equation [1] (4.24):

$$\frac{d(C_2)_{25}(t)}{dt} = -\kappa_{28}(C_2)_{85}(t) \quad , \quad t > 0 \tag{4.6}$$

$$\kappa_{28} = i\omega_{25} + \gamma_{25} \tag{4.7}$$

γ is the dissipation matrix, the space-time integral over the memory function of the process which is defined with the linear projection operator employed here. In [2] it is emphasized in connection with formula (3.18) there, that in general one has to distinguish this from the corresponding quantities defined with the multilinear projection operator defined there. For the limited purpose of the present paper, this difference can be ignored. The condition $t > 0$ in (4.6) is essential, since at $t = 0$ the time derivative of C_2 is discontinuous: While from the definition of C_2 and the conservation relations we find $\frac{d(C_2)_{25}}{dt}|_{t=0} = -i\omega_{25}$, from (4.6) one concludes $\frac{d(C_2)_{25}}{dt}|_{t=0+} = -\kappa_{25}$. - (4.6) is introduced into (4.5), and the integration parameter t' is transformed:

$$(K_{21})_{25}(t) = \kappa_{8,11} \int_0^t dt' (K_{21})_{28}(t')(C_2)_{11,5}(t-t') + \kappa_{2,11}(C_2)_{11,5}(t) \quad , \quad t > 0 \tag{4.8}$$

Differentiation with respect to time and insertion of (4.8),(4.6) yields:

$$\begin{aligned}
\frac{d(K_{21})_{25}(t)}{dt} &= -\kappa_{14,5} \{ [(K_{21})_{2,14}(t) - \kappa_{2,11}(C_2)_{11,14}(t)] + \kappa_{2,11}(C_2)_{11,14}(t) \} + \kappa_{85}(K_{21})_{28}(t) \\
&= 0 \quad , \quad t > 0
\end{aligned} \tag{4.9}$$

Thus, for $t > 0$, K_{21} is a constant. The value is found from (4.8) by taking the time limit $t = 0_+$:

$$(K_{21})_{25} = \kappa_{25} \quad , \quad t > 0 \tag{4.10}$$

For calculating the properties of K_{22} , we need an operator identity similar to (4.4):

$$e^{(1-\mathcal{P})\mathcal{L}t} = e^{\mathcal{L}t} - \int_0^t dt' e^{(1-\mathcal{P})\mathcal{L}t'} \mathcal{P} \mathcal{L} e^{\mathcal{L}(t-t')} \tag{4.11}$$

Both formulas can be found from more general identities in [3]. The calculation is quite similar to that of K_{21} , and the result is:

$$\frac{d(K_{22})_{25}(t)}{dt} = 0 \quad , \quad t > 0 \tag{4.12}$$

$$(K_{22})_{25} = \delta_{25} \quad , \quad t > 0 \tag{4.13}$$

Introducing these results into (4.3), we obtain:

$$\frac{d(K_2)_{25}(t)}{dt} = 0, \quad t > 0 \quad (4.14)$$

$$(K_2)_{25} = -\gamma_{25}, \quad t > 0 \quad (4.15)$$

Combining (4.15) and (4.1) yields:

$$(K_2)_{25}(t) = -\gamma_{25}\Theta(t), \quad t \geq 0 \quad (4.16)$$

$\Theta(t)$ is the step function. By Differentiation:

$$\frac{d(K_2)_{25}(t)}{dt} = -\gamma_{25}2\delta(t), \quad t \geq 0 \quad (4.17)$$

It is understood that the dimension of the delta function corresponds to that of its argument; always the same symbol δ is used. The factor 2 is necessary since the delta function has its peak at the boundary of the definition range of K_2 . - Formula (4.17) constitutes the essential difference to the first version of this paper, where the result (4.9) stated $\frac{d(K_2)_{25}(t)}{dt} = 0, t \geq 0$. By inserting (4.17) into (3.10) and evaluating the delta function:

$$(D_{2f})_1(t) = -\beta^{\frac{1}{2}}\rho^{\frac{3}{2}}\frac{\gamma_{25}}{(2\pi)^6} \int d\mathbf{q} \int d\mathbf{q}' \int_0^t dt' (K_3)_{153}(t-t')u_2(t')u_3(t') \quad (4.18)$$

Since the hydrodynamic velocity varies on a much longer time scale than the equilibrium correlation function, it is again possible to apply a Markovian approximation:

$$(D_{2f})_1(t) = \beta^{\frac{1}{2}}\rho^{\frac{3}{2}}\frac{1}{(2\pi)^6} \int d\mathbf{q} \int d\mathbf{q}' (N_f)_{123}u_2(t)u_3(t) \quad (4.19)$$

$$(N_f)_{123} = -\gamma_{25} \int_0^\infty dt' (K_3)_{153}(t') \quad (4.20)$$

5 Calculation of K_3

In contrast to the first version of this paper, we now need to calculate the correlation function K_3 . We again use the identity (4.4); with a calculation which parallels [1] (4.10) to (4.12) we obtain a formula for K_3 :

$$(K_3)_{123}(t) = -\gamma_{14}\langle [e^{\mathcal{L}t} h_4] h_2^* h_3^* \rangle_0 + \langle [e^{\mathcal{L}t} (i\mathbf{k}\hat{r})_1] h_2^* h_3^* \rangle_0 \quad (5.1)$$

The first term contains the non-projected single-time triple correlation function:

$$(C_3)_{123}(t) = \langle [e^{\mathcal{L}t} h_1] h_2^* h_3^* \rangle_0 \quad (5.2)$$

The second term can be transformed by the relation (4.2). We obtain from (5.1):

$$(K_3)_{123}(t) = -\kappa_{14}(C_3)_{423}(t) - \frac{d(C_3)_{123}(t)}{dt} \quad (5.3)$$

We switched to reduced correlations since this is more suitable for the following calculation. - As has been stated in [1], for C_3 expression (4.20) has been derived by multilinear mode coupling theory:

$$(C_3)_{123}(t) = (C_2)_{14}(t) \tilde{J}_{423} - \int_0^t dt' (C_2)_{14}(t-t') i k_d S_{456d} (C_2)_{52}(t') (C_2)_{63}(t') \quad (5.4)$$

J is given in [1] (4.23). For K_3 , we then find:

$$(K_3)_{123}(t) = i k_d S_{156d} (C_2)_{52}(t) (C_2)_{63}(t) \quad (5.5)$$

The solution of (4.6) to the initial condition $(C_2)_{14}(0) = \delta_{14}$ is:

$$(C_2)_{14}(t) = e^{-\kappa_{14}t} \quad (5.6)$$

This is inserted into (5.5); by integration we obtain for N_f (4.20):

$$(N_f)_{123} = -\gamma_{25}(\kappa_{58}\delta_{36} + \delta_{58}\kappa_{36})^{-1}ik_d S_{186d} \quad (5.7)$$

For insertion into (4.19), we may replace $(N_f)_{123}$ by the symmetric form $\frac{1}{2}((N_f)_{123} + (N_f)_{132})$ which we denote by the same symbol:

$$\begin{aligned} (N_f)_{123} &= -\frac{1}{2}(\gamma_{25}\delta_{36} + \delta_{25}\gamma_{36})(\kappa_{58}\delta_{69} + \delta_{58}\kappa_{69})^{-1}ik_d S_{189d} \\ &= -\frac{1}{2}ik_d S_{123d} + \frac{1}{2}(i\omega_{25}\delta_{36} + \delta_{25}i\omega_{36})(\kappa_{58}\delta_{69} + \delta_{58}\kappa_{69})^{-1}ik_d S_{189d} \end{aligned} \quad (5.8)$$

When this is introduced into (4.19), it is seen that the second term vanishes because $\omega_{25} = \check{\omega}_5 q_2$ ($\check{\omega}_5$ certain constants), and the incompressibility condition reads $q_2 u_2 = 0$. Thus, for the relevant part of N_f , we have:

$$(N_f)_{123} = -(2\pi)^3 \delta(\mathbf{k} - \mathbf{q} - \mathbf{q}') \frac{1}{2} ik_d S_{123d} \quad (5.9)$$

When we compare with (3.7), we obtain from (3.2):

$$D_2 = 0 \quad (5.10)$$

Thus, with the recalculation of K_2 (4.16), we now obtain the result that the second-order part of the friction force vanishes.

6 Stationary processes

We shortly turn to the earlier paper [1], where we considered stationary processes. When the calculation is performed in Fourier space and orthonormal variables are introduced, inserting (A9) into (4.1) and importing this into (3.2) of that paper yields the consecutive formula für D_{2f} :

$$(D_{2f})_1 = \beta^{\frac{1}{2}} \rho^{\frac{3}{2}} \frac{1}{(2\pi)^6} \int d\mathbf{q} \int d\mathbf{q}' k_c q_d \int_0^\infty dt' \int_0^\infty dt'' \langle \left[\frac{d}{dt'} e^{(1-\mathcal{P})\mathcal{L}t'} \mathcal{P} h_3^* e^{(1-\mathcal{P})\mathcal{L}t''} \hat{r}_{1c} \right] \hat{r}_{2d}^* \rangle_0 u_2 u_3 \quad (6.1)$$

As in [1], the projection operation is performed:

$$(D_{2f})_1 = \beta^{\frac{1}{2}} \rho^{\frac{3}{2}} \frac{k_c q_d}{(2\pi)^6} \int d\mathbf{q} \int d\mathbf{q}' \int_0^\infty dt' \int_0^\infty dt'' \langle [e^{(1-\mathcal{P})\mathcal{L}t''} \hat{r}_{1c}] h_3^* h_3^* \rangle_0 \frac{d}{dt'} \langle [e^{(1-\mathcal{P})\mathcal{L}t'} h_5] \hat{r}_{2d}^* \rangle_0 u_2 u_3 \quad (6.2)$$

It has been taken into account that we have:

$$\langle [e^{(1-\mathcal{P})\mathcal{L}t''} \hat{r}_{1c}] h_3^* \rangle_0 = \langle [e^{\mathcal{L}(1-\mathcal{P})t''} \hat{r}_{1c}] (1 - \mathcal{P}) h_3^* \rangle_0 = 0 \quad (6.3)$$

Definitions (3.11), (3.12) of the present paper are introduced:

$$\begin{aligned} (D_{2f})_1 &= -\beta^{\frac{1}{2}} \rho^{\frac{3}{2}} \frac{1}{(2\pi)^6} \int d\mathbf{q} \int d\mathbf{q}' u_2 u_3 \int_0^\infty dt'' (K_3)_{153}(t'') \int_0^\infty dt' \frac{d(K_2)_{52}(t')}{dt''} \\ &= -\beta^{\frac{1}{2}} \rho^{\frac{3}{2}} \frac{1}{(2\pi)^6} \int d\mathbf{q} \int d\mathbf{q}' u_2 u_3 \int_0^\infty dt'' (K_3)_{153}(t'') \left[\lim_{t' \rightarrow \infty} (K_2)_{52}(t') - (K_2)_{52}(0) \right] \end{aligned} \quad (6.4)$$

It has been assumed in [1] that for large t the factor variables of K_2 become statistically independent; this led to $\lim_{t' \rightarrow \infty} (K_2)_{52}(t') = 0$. But as we see from (4.15), for K_2 this assumption is not true. When the correct formula is incorporated, the calculation leads to the final result (5.10).

7 Summary

As is stated in the introduction, $D_2 = 0$ ensures that the Navier-Stokes equation is obtained correctly as second-order velocity approximation of the mean momentum equation derived by projection operator technique.

A Appendix: Calculation of the functional derivative

The kernel function (2.3) depends on b_e 4-fold, namely, in the formula for the local equilibrium density ρ_L , in \mathcal{P} contained in \hat{s}_{ac} and \hat{s}_{bd} , and in the operator \mathcal{G} . For abbreviation, the formula for the derivative is written:

$$\frac{\delta R_{abcd}(\mathbf{x}, \mathbf{x}', t, t')}{\delta b_e(\mathbf{x}'', t'')} = \sum_{i=1}^4 \left[\frac{\delta R}{\delta b} \right]^{(i)} \quad (\text{A.1})$$

In the first three of these, the time dependence of R is parametric via the time dependence of ρ_L , at the time instant t or t' . In these cases, the time-dependent derivative is equal to the corresponding stationary derivative times $\delta(t'' - t)$ or $\delta(t'' - t')$. The stationary derivatives are given in [1] (A3) to (A5). We still have to take these formulas at $\mathbf{u} = 0$; then, ρ_L switches to ρ_0 , the probability density of total equilibrium (for a given density and temperature), and therefore $\langle \rangle_{L,t}$ to $\langle \rangle_0$, the equilibrium expectation; \mathcal{P} reduces to \mathcal{P}_0 , the corresponding total equilibrium projection operator; \hat{s}_{ac} to $(\hat{s}_0)_{ac}$, the flux density projected by \mathcal{P}_0 ; δp_e to p_e , and $\mathcal{G}(t', t)$ to $e^{(1-\mathcal{P}_0)\mathcal{L}(t-t')}$. We obtain:

$$\left[\frac{\delta R_{abcd}}{\delta b_e} \right]_{\mathbf{u}=0}^{(1)} = -\delta(t'' - t')\beta \langle [e^{\mathcal{L}(1-\mathcal{P}_0)(t-t')} (\hat{s}_0)_{ac}(\mathbf{x})] p_e(\mathbf{x}'') (\hat{s}_0)_{bd}(\mathbf{x}') \rangle_0 \quad (\text{A.2})$$

$$\left[\frac{\delta R_{abcd}}{\delta b_e} \right]_{\mathbf{u}=0}^{(2)} = \delta(t'' - t')\beta \langle [e^{\mathcal{L}(1-\mathcal{P}_0)(t-t')} (\hat{s}_0)_{ac}(\mathbf{x})] \mathcal{P}_0 p_e(\mathbf{x}'') (\hat{s}_0)_{bd}(\mathbf{x}') \rangle_0 \quad (\text{A.3})$$

$$\left[\frac{\delta R_{abcd}}{\delta b_e} \right]_{\mathbf{u}=0}^{(3)} = \delta(t'' - t)\beta \langle [e^{\mathcal{L}(1-\mathcal{P}_0)(t-t')} \mathcal{P}_0 p_e(\mathbf{x}'') (\hat{s}_0)_{ac}(\mathbf{x})] (\hat{s}_0)_{bd}(\mathbf{x}') \rangle_0 \quad (\text{A.4})$$

We have:

$$\begin{aligned} \langle [e^{\mathcal{L}(1-\mathcal{P}_0)t} \mathcal{P}_0 A] (1 - \mathcal{P}_0) B \rangle_0 &= \langle [(1 - \mathcal{P}_0) e^{\mathcal{L}(1-\mathcal{P}_0)t} \mathcal{P}_0 A] (1 - \mathcal{P}_0) B \rangle_0 \\ &= \langle [e^{(1-\mathcal{P}_0)\mathcal{L}t} (1 - \mathcal{P}_0) \mathcal{P}_0 A] (1 - \mathcal{P}_0) B \rangle_0 \\ &= 0 \end{aligned} \quad (\text{A.5})$$

From this we find:

$$\left[\frac{\delta R_{abcd}}{\delta b_e} \right]_{\mathbf{u}=0}^{(3)} = 0 \quad (\text{A.6})$$

The remaining two parts yield the parametric part of the functional derivative:

$$\begin{aligned} \left[\frac{\delta R_{abcd}}{\delta b_e} \right]_p &= \left[\frac{\delta R_{abcd}}{\delta b_e} \right]_{\mathbf{u}=0}^{(1)} + \left[\frac{\delta R_{abcd}}{\delta b_e} \right]_{\mathbf{u}=0}^{(2)} \\ &= -\delta(t'' - t')\beta \langle [e^{\mathcal{L}(1-\mathcal{P}_0)(t-t')} (\hat{s}_0)_{ac}(\mathbf{x})] (1 - \mathcal{P}_0) p_e(\mathbf{x}'') (\hat{s}_0)_{bd}(\mathbf{x}') \rangle_0 \\ &= -\delta(t'' - t')\beta \langle [e^{(1-\mathcal{P}_0)\mathcal{L}(t-t')} (\hat{s}_0)_{ac}(\mathbf{x})] (\hat{s}_0)_{bd}(\mathbf{x}') p_e(\mathbf{x}'') \rangle_0 \end{aligned} \quad (\text{A.7})$$

Note that in the 2nd step, in the exponent the sequence of operators is reversed; compare (A.5) for a similar operation.

The 4th part of the derivative is defined:

$$\left[\frac{\delta R_{abcd}}{\delta b_e(\mathbf{x}'', t'')} \right]^{(4)} = \beta \langle \left[\frac{\delta \mathcal{G}(t', t)}{\delta b_e(\mathbf{x}'', t'')} (1 - \mathcal{P}(t)) s_{ac}(\mathbf{x}) \right] (1 - \mathcal{P}(t')) s_{bd}(\mathbf{x}') \rangle_{L, t'} \quad (\text{A.8})$$

By temporarily approximating the Integral in (2.6) by a sum, one finds for the derivative of $\mathcal{G}(t', t)$:

$$\frac{\delta \mathcal{G}(t', t)}{\delta b_e(\mathbf{x}'', t'')} = \int_{t'}^t d\tau \mathcal{G}(t', \tau) \frac{\delta(\mathcal{L}(1 - \mathcal{P}(\tau)))}{\delta b_e(\mathbf{x}'', t'')} \mathcal{G}(\tau, t) \quad (\text{A.9})$$

Moreover, for the middle factor of the integrand which depends parametrically on τ , we have:

$$\frac{\delta(\mathcal{L}(1 - \mathcal{P}(\tau)))}{\delta b_e(\mathbf{x}'', t'')} = \delta(t'' - \tau) \mathcal{L} \mathcal{P}(t'') \delta p_e(\mathbf{x}'', t'') (1 - \mathcal{P}(t'')) \quad (\text{A.10})$$

This is introduced into (A.9). The following structure arises:

$$\int_{t'}^t d\tau \delta(t'' - \tau) F(t'', \tau) = \Theta(t'' - t') \Theta(t - t'') F(t'', t'') \quad (\text{A.11})$$

with $\Theta(t)$ being the step function:

$$\Theta(t) = \begin{cases} 0, & t \leq 0 \\ 1, & t > 0 \end{cases} \quad (\text{A.12})$$

We obtain:

$$\frac{\delta \mathcal{G}(t', t)}{\delta b_e(\mathbf{x}'', t'')} = \Theta(t'' - t') \Theta(t - t'') \mathcal{G}(t', t'') \mathcal{L} \mathcal{P}(t'') \delta p_e(\mathbf{x}'', t'') (1 - \mathcal{P}(t'')) \mathcal{G}(t'', t) \quad (\text{A.13})$$

This is introduced into (A.8):

$$\begin{aligned} \left[\frac{\delta R_{abcd}}{\delta b_e(\mathbf{x}'', t'')} \right]^{(4)} &= \beta \Theta(t'' - t') \Theta(t - t'') \times \\ &\times \langle [\mathcal{G}(t', t'') \mathcal{L} \mathcal{P}(t'') \delta p_e(\mathbf{x}'', t'') (1 - \mathcal{P}(t'')) \mathcal{G}(t'', t) \hat{s}_{ac}(\mathbf{x}, t)] \hat{s}_{bd}(\mathbf{x}', t') \rangle_{L, t'} \end{aligned} \quad (\text{A.14})$$

For $\mathbf{u} = 0$, this reads:

$$\begin{aligned} \left[\frac{\delta R_{abcd}}{\delta b_e(\mathbf{x}'', t'')} \right]_{\mathbf{u}=0}^{(4)} &= \beta \Theta(t'' - t') \Theta(t - t'') \times \\ &\times \langle [e^{\mathcal{L}(1-\mathcal{P}_0)(t''-t')} \mathcal{L} \mathcal{P}_0 p_e(\mathbf{x}'') (1 - \mathcal{P}_0) e^{\mathcal{L}(1-\mathcal{P}_0)(t-t'')}] (\hat{s}_0)_{ac}(\mathbf{x}) (\hat{s}_0)_{bd}(\mathbf{x}') \rangle_0 \end{aligned} \quad (\text{A.15})$$

After some manipulations, the result is:

$$\begin{aligned} \left[\frac{\delta R_{abcd}}{\delta b_e(\mathbf{x}'', t'')} \right]_{\mathbf{u}=0}^{(4)} &= \beta \Theta(t'' - t') \Theta(t - t'') \times \\ &\times \langle [e^{(1-\mathcal{P}_0)\mathcal{L}(t''-t')} (1 - \mathcal{P}_0) \mathcal{L} \mathcal{P}_0 p_e(\mathbf{x}'') e^{(1-\mathcal{P}_0)\mathcal{L}(t-t'')}] (\hat{s}_0)_{ac}(\mathbf{x}) (\hat{s}_0)_{bd}(\mathbf{x}') \rangle_0 \\ &= -\beta \Theta(t'' - t') \Theta(t - t'') \times \\ &\times \langle \left[\frac{d}{dt'} e^{(1-\mathcal{P}_0)\mathcal{L}(t''-t')} \mathcal{P}_0 p_e(\mathbf{x}'') e^{(1-\mathcal{P}_0)\mathcal{L}(t-t'')} \right] (\hat{s}_0)_{ac}(\mathbf{x}) (\hat{s}_0)_{bd}(\mathbf{x}') \rangle_0 \end{aligned} \quad (\text{A.16})$$

References

- [1] J. Piest: Problem with the derivation of the Navier-Stokes equation by means of Zwanzig-Mori projection technique of statistical mechanics. arXiv 0711.2790v1
- [2] J. Schofield, R. Lim, I. Oppenheim, Physica A181 (1992), 89
- [3] Zubarev, D.; Mozorov, V.; Röpke, G: Statistical mechanics of nonequilibrium processes. Vol. 1, Abschn. 2B